Modeling of Solid Oxide Electrolysis Cells – Physics-based Impedance Analysis of Mixed Ionic Electronic Conducting Electrodes

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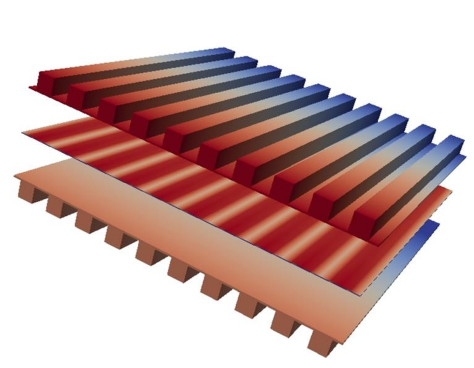
Motivation

With increasing penetration of renewable energy into the energy system, the number of periods where the power generation exceeds the demand rises.
In the KOPERNIKUS Project Power-to-X different technologies to convert and store this surplus electricity are investigated. Solid oxide electrolysis cells (SOECs) are capable to efficiently produce syngas (H_2 + CO) via co-electrolysis of water and carbon dioxide. The obtained syngas can be converted into e.g. liquid fuels via the Fischer-Tropsch-synthesis in subsequent processes.
To understand how operating conditions like temperature, pressure and fuel composition influence the performance, the product composition (H_2/CO-ratio) and degradation of SOECs, a physics-based cell-level model has been developed. With this model, the cell behavior is rationalized. In perspective, the model will be applied for the virtual design of SOECs to reduce degradation phenomena and improve performance.

Modeling approach – NEOPARD-X[1]

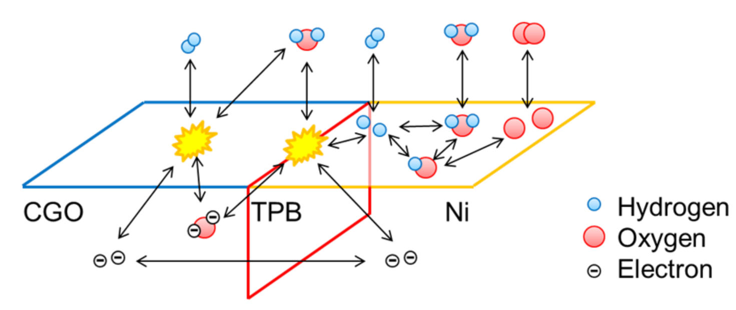
Transient and macro-homogeneous formulations of mass-, charge- and energy balances:



$$\frac{\partial \xi^i}{\partial t} + \nabla \cdot \Psi^i - q^i = 0$$

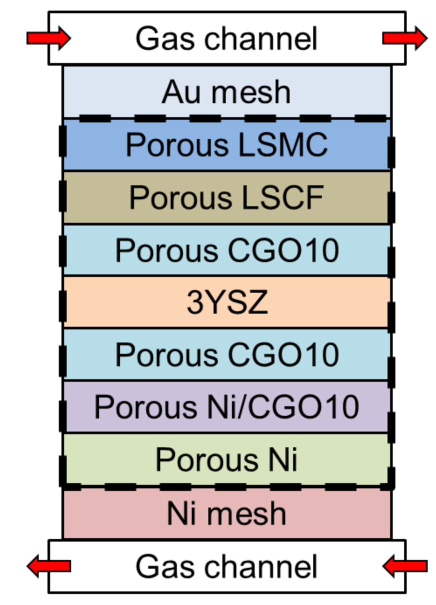
Mass:
- Darcy's law in combination with Stefan-Maxwell- and Knudsen diffusion in the porous electrodes

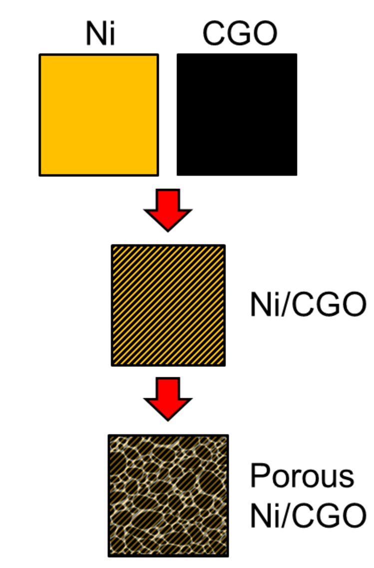
Charge:
- Ohm's law for electrical- and ionic currents
- Half cell reactions are modeled using thermodynamically consistent elementary kinetics



Energy:
- Energy transport due to mass- and charge transport
- Heat formation due to ohmic heating
- Heat formation due to elementary reactions

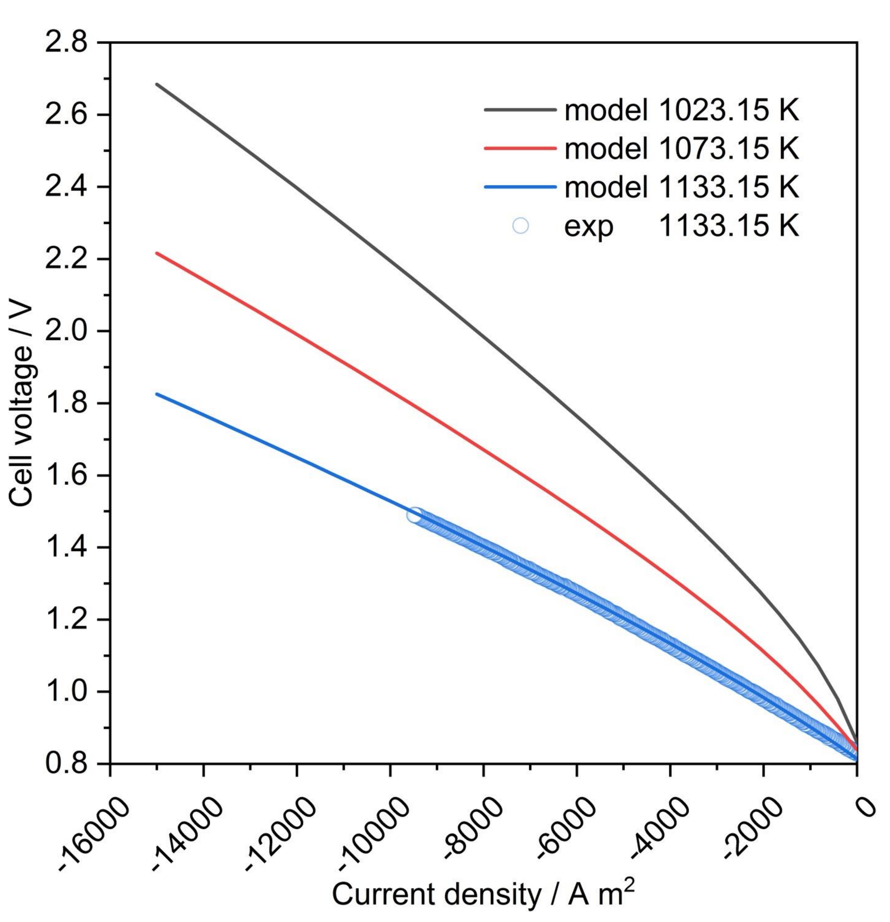
Material modeling:
- Derivation of effective properties from bulk properties and structural parameters





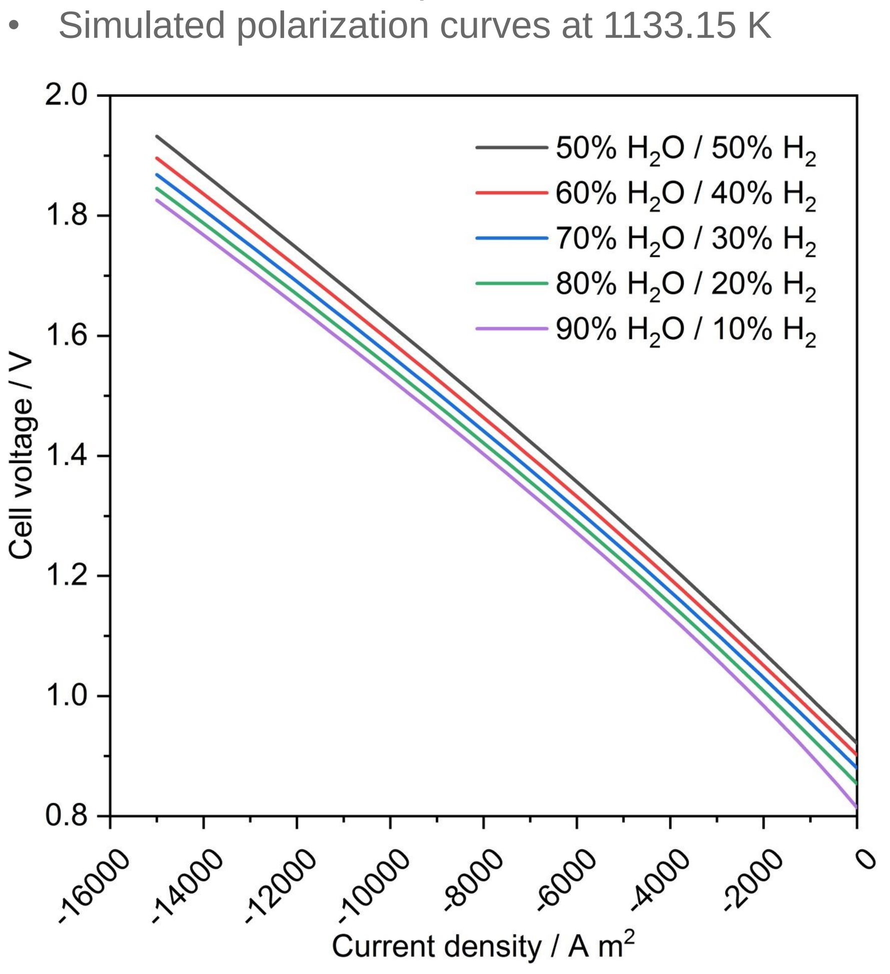
Results

Towards model validation:
- Comparison of simulated and experimental polarization curve at various temperatures:



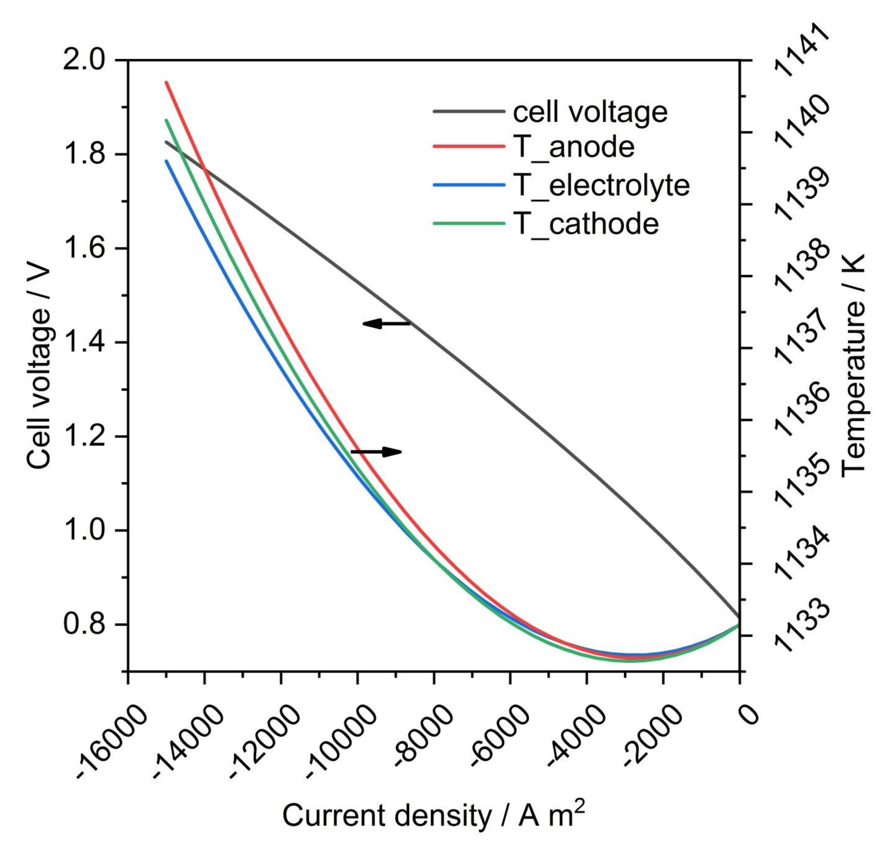
- ➢ Excellent agreement between model and experiment (for now only in one condition due to test bench issues)
- ➢ Model predicts increasing resistance with decreasing temperature, mainly due to ohmic resistance of the electrolyte

Influence of the fuel composition:
- Simulated polarization curves at 1133.15 K



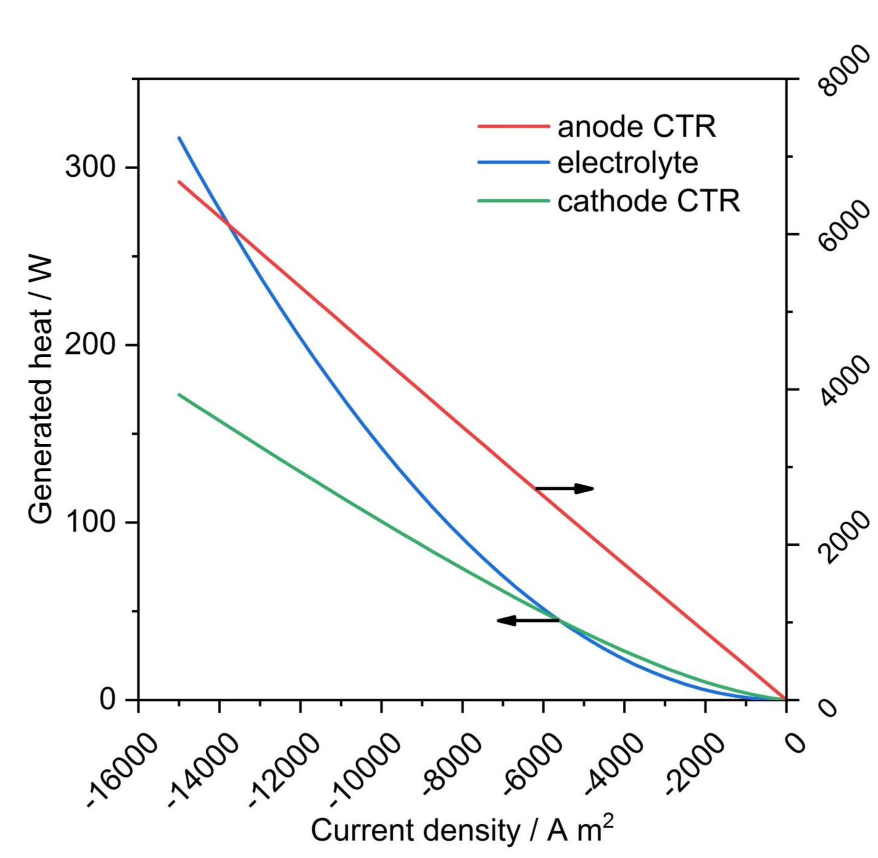
- ➢ Model predicts increasing cell voltage with decreasing water content

Thermo-neutral voltage:
- Simulated polarization curve and average temperature of the electrodes and electrolyte:



- ➢ Endo- and exothermal cell behavior depending on the cell voltage is represented correctly by the model

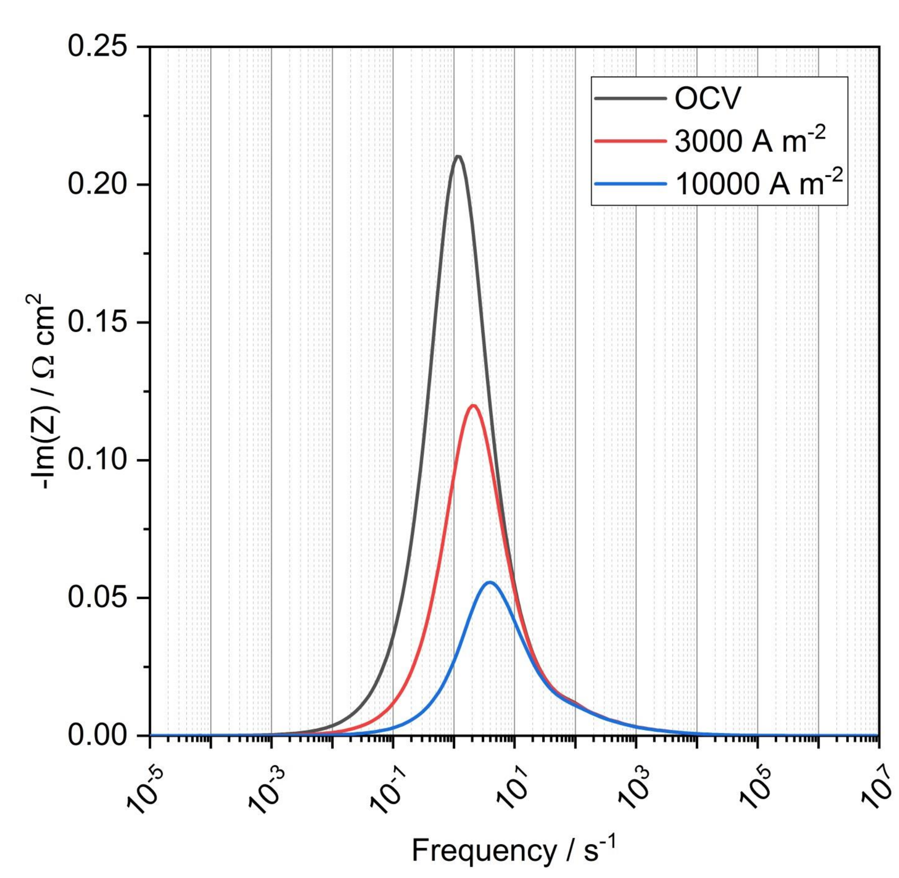
Contributions of charge transfer reactions in the electrodes and ohmic heating in the electrolyte to the heat formation:
- Depicted: heat generated due to electrical power



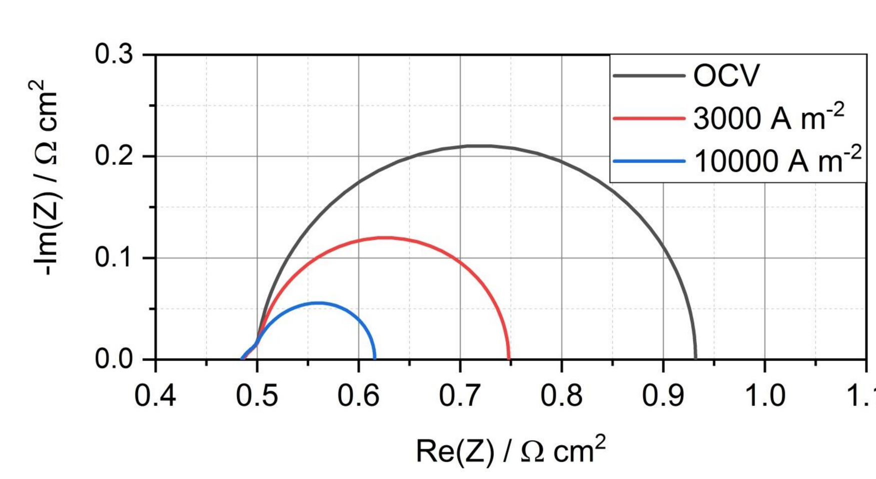
- ➢ With the current parametrization, the majority of the heat is generated at the cathode
- ➢ $q^{heat}_{electrolyte} \sim i^2$

Physics-based impedance analysis:
- Rapid calculation of the impedance with the current/voltage step method[2]
- Resolution of a huge frequency range with a single transient simulation
- Allows interpretation of impedance spectra based on complex theoretical models

Bode plot for the imaginary part of the impedance at OCV, 0.3 A cm^{-2} and 1 A cm^{-2}:



Nyquist plot at OCV, 0.3 A cm^{-2} and 1 A cm^{-2}:



- ➢ Decreasing slope of the polarization curve is due to increasing kinetics with current density
- ➢ Change of ohmic resistance with current density (and therefore temperature) is negligible
- ➢ Transport limitation under the given operating conditions is negligible

References

[1]: Futter et al., JPS 391 (2018), 148-161.
[2]: Bessler, JES 154 (2007), B1186-B1191.

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KOPERNIKUS PROJEKTE P2X Die Zukunft unserer Energie

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